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First International Conference on Highly Organized Catalytic Systems

The First International Conference on Highly Organized Catalytic Systems (HOCS-1) was held on June 24–27, 2002, in Chernogolovka. The conference was organized by the Institute of Problems of Chemical Physics, Russian Academy of Sciences, and the Chemistry Department of Moscow State University. The Russian Foundation for Basic Research, the Ministry of Science and Technology of the Russian Federation, the Council on Catalysis of the Russian Academy of Sciences, and Haldor Topsøe A/S provided substantial financial and organizational support. Thirty-five plenary lectures and oral talks, as well as 64 posters, were presented. Over 140 researchers from various regions of Russia and other countries (Austria, Great Britain, Germany, Denmark, Kazakhstan, Poland, Finland, France, Japan, and others) took part in the conference.

Although this is the first international conference, such conferences have rather a long history and can be considered traditional. The two preceding meetings were Russian (in 1998 and 2000), and the last one joined researchers from seven countries. Before that there were two seminars on highly organized catalytic systems held in Moscow.

Experience of the four preceding meetings led the organizers to conduct the conference on an international scale. Indeed, despite many European and international meetings on catalysis, there has been none that focused on the problems of structural and chemical organization, self-organization, and the directed evolution of complex catalytic systems, although these problems are central to modern catalysis. Without advancement in this direction, recent progress in creating new highly efficient catalysts for a wide variety of processes would have been impossible. It is characteristic that both Russian and foreign participants noted the uniqueness and urgency of the conference topics when discussing the overall results this meeting.

Advances in the area of highly organized catalytic systems determined the variety of problems discussed at the conference, but some key areas can be highlighted. Thus, catalysis by clusters and nanocomposites fills one of the most important places. These problems were considered in a number of interesting talks, including the lecture of Academician Moiseev. He analyzed in detail the trends in the coordination chemistry of nanoparticles and clusters, which have now become an important subdiscipline of coordination chemistry. This lecture considered the main trends in this area using mostly platinum group metal cluster complexes as examples and demonstrated modern methodological approaches to studies of this sort. This lecture was complemented by Professor Schubert (Technological University, Vienna), who provided a detailed overview of sol-gel technology, one of the main methods for creating nanosized metallic and metal oxide catalysts. In the talk of Rostovshchikova *et al.* (Moscow State University, Ioffe Physicotechnical Institute) a new method was proposed based on the directed formation of ensembles of interacting nanoparticles on the surface of supports or polymeric matrices for the design of nanocluster metal catalysts. In the report of Loktev *et al.* (Moscow State University), synergistic effects in the catalysis by nanoclusters in practically important hydrodechlorination reactions were analyzed. The specific features of magnesium clusters, which appeared to be similar to some transition metal complexes in their catalytic properties, were considered in the report by Tyurina (Moscow State University). Another not less important area widely discussed at the conference is associated with catalysis by highly organized metal oxides and supported metal complexes. The mechanism of action of metal porphyrin complexes in the oxidation of cycloalkanes was considered by Bagrii *et al.* (Topchiev Institute of Petrochemical Synthesis, Russian Academy of Sciences). Tsodikov *et al.* (Topchiev Institute of Petrochemical Synthesis) devoted his talk to a very interesting manifestation of the molecular-sieve effect in the oxyethylation of alcohols on doped titanium phosphorus oxide. Volodin (Boreskov Institute of Catalysis, Siberian Division, Russian Academy of Sciences) proposed an original method for the formation of catalysts based on low-valence metals on oxide supports. This method was called spin design. The problems of asymmetric catalysis on immobilized platinum derivatives were considered in the report of Toukoniitty *et al.* (University of Abo, Finland). The lecture of Candy and Basset (Institute of Catalysis, Villerban, France) treated the same group of problems and provided an overview of the surface chemistry of organometallic compounds applied to their catalytic properties. Considerable attention was given at the conference to the problems of the structural organization in acid–base catalysis. The detailed lecture of Professor Ai (Niigata Technological University, Japan) showed that acid–base interactions may play a key role in oxidative dehydrogenation processes. Academician Kazanskii (Zelinskii Institute of Organic Chemistry) delivered a lecture and analyzed the structural organization of olefin alkylation by

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isoalkanes. The directed use of the structural features of heteropoly acids in catalytic acylation was considered by Kaur *et al.* (Liverpool University, Great Britain). The role of acid catalysis in the homolytic processes of N–N bond cleavage was analyzed in the talk of Varlamov (Institute of Problems of Chemical Physics, Russian Academy of Sciences). Catalysis by micellar systems was considered by Oehme *et al.* (Institute of Organic Catalysis in Rostock, Germany) and a group of authors led by Kasaikina (Semenov Institute of Chemical Physics, Russian Academy of Sciences). Two reports devoted to the theoretical studies of highly organized catalytic systems are notable. Shestakov (Institute of Problems of Chemical Physics, Russian Academy of Sciences) carried out the quantum chemical modeling of the Mo cofactor and Ustynyuk (Moscow State University) calculated the transition metal complexes with macrocyclic ligands considered as models of enzyme active centers. The problems of applied catalysis were not the focus of the conference, but several talks revealed the complex relationship between the level of understanding the mechanism of the role of organization of catalytic systems and practical achievements. Thus, papers by Herbst (Haldor Topsøe A/S, Denmark) and Kochubei (Boreskov Institute of Catalysis, Siberian Division, Russian Academy of Sciences) devoted to the properties and directed formation of cluster molybdenum sulfide systems were closely related to the processes of hydrorefining. CO oxidation on structurally organized catalysts (the lecture by Jaeger from the Institute of General and Physical Chemistry, Bremen, Germany) and the mechanisms of catalytic conversion of C_1 molecules (the lecture by Rozovskii from the Institute of Petrochemical Synthesis, Russian Academy of Sciences) cannot be considered separately from practical needs. In the latter lecture, the author provided new supporting arguments for the ideology recently developed by him that rejects the old scheme of heterogeneously catalyzed reactions (adsorption–reaction–desorption) and considers these reactions as a set of bimolecular processes with the participation of the substrates and surface complexes.

Of course one conference with a limited number of participants cannot analyze all the trends in the progress of research in the area of highly organized catalytic systems, but some conclusions can be drawn. First, we see a strengthening interweaving of methods and ideas from various fields of catalysis. In many cases, the results on seemingly typical metal complex catalysts cannot be explained without considering the impact of acid–base interactions. At the same time, some systems based on nontransition metals show properties that are characteristic of transition metals. Many examples confirm the necessity of considering a supported catalyst as a unit catalytic complex; its separation into the active site and the inert support usually does not provide the correct understanding of the mechanism of functioning of the whole system. Along with the use of modern physical methods, the applicability domain of computational methods is expanding. In computational catalysis the role of density functional theory will probably increase, since this theory combines the relative simplicity of calculations and the rather good description of very complex systems. A trend toward close relationships between the objects of studies and practical technologies is seen. This concerns large-scale syntheses and (to a greater extent) fine organic synthesis, pharmaceutics, and other areas directed at the synthesis of small-scale valuable target products. As for organizational matters, we clearly see growing scientific cooperation, as in many other areas of chemistry: with the exception of review reports, most of the contributions were the results of collaborative research from several institutions and different regions (often from different countries).

In general, the participants of the conference positively evaluated its results and expressed their confidence in the need for regular conferences of this sort. The specific date of the next conference will be determined later, taking into account the schedule of other international meetings on catalysis. It was requested to hold the Second International Conference on Highly Organized Catalytic Systems (HOCS-2) in 2004 in Moscow.

Proceedings of the First International Conference on Highly Organized Catalytic Systems will be published in the next issue of the journal.

V. V. Smirnov